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An Efficient Method for Evaluating the J(β,θ,a,b) Integral

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ABSTRACT

This report describes a new technique for evaluating the generalized form of the resonance integral which allows the multilevel formalism. By taking advantage of the asymptotic behavior of the Doppler-broadened line shape functions, the technique of rational transformation is introduced. The Gauss-Jacobi quadrature is used to evaluate the integral with the transformed integrand. The detailed description of this technique and its mathematical justifications are given.

INTRODUCTION

The integral $J\left(\beta_k,\theta_k,a_k,b_k\right)$ represents a generalized form of the usual J-integral which arises: (1) when the effect of the interference scattering cross section in the single-level formulation is included; or (2) when the multilevel formalism is used. $J\left(\beta_k,\theta_k,a_k,b_k\right)$ is defined as

$$J\left(\beta_k,\theta_k,a_k,b_k\right) = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\psi\left(\theta_k,x_k\right) + b_k\chi\left(\theta_k,x_k\right)}{\beta_k + 2a_k x_k + \psi\left(\theta_k,x_k\right)}\, dx_k \,, \tag{1}$$

where the parameters are defined according to how the cross sections are formulated.[1,2] Physically, it is equivalent to the resonance integral of an "isolated" resonance excluding the effect of mutual self-shielding due to the neighboring resonances when the NR-approximation is assumed. In other words, it has precisely the same physical meaning of the usual J-integral.

In the single-level formulation, b_k is set to be zero. Parameters β_k and a_k can be defined slightly differently in the resolved and the unresolved resonance regions to be consistent with the data in the ENDF/B file. For the resolved resonance region, a_k and β_k are defined as

$$a_k = \sqrt{\beta_k \cdot g_J \cdot \frac{\Gamma_{nk}}{\Gamma_k} \cdot \frac{\sigma_{pa}}{\sigma_p}} \,, \tag{2}$$

where

$$\beta_k = \sigma_p/\sigma_{0k}$$

σ_{pa} = potential scattering cross section of the absorber under consideration (barns)

$\sigma_p = \Sigma_t/N$ or Σ_t^{eq}/N (barns/atom).

For the unresolved energy region, parameters β_k and a_k can be defined as

$$a_k = 1/2 \tan 2\delta_\ell \tag{3}$$

and

$$\beta_k = \sigma_p \Big/ \left(\sigma_{0k} \cos 2\delta_\ell\right) \quad \text{(or the equivalent } \sigma_p\text{)} , \tag{4}$$

where

$$\delta_\ell = \arctan \left[\frac{j_\ell(R/\lambda\!\!\!^{-})}{n_\ell(R/\lambda\!\!\!^{-})}\right] \tag{5}$$

$$\delta_0 = R/\lambda\!\!\!^{-} \tag{6}$$

$$\delta_1 = R/\lambda\!\!\!^{-} - \arctan (R/\lambda\!\!\!^{-}) \tag{7}$$

$$\delta_2 = R/\lambda\!\!\!^{-} - \arctan \left[\frac{3R/\lambda\!\!\!^{-}}{3 - (R/\lambda\!\!\!^{-})^2}\right] , \tag{8}$$

and j_ℓ and n_ℓ are the spherical Bessel and Neumann functions, respectively.

The resonance integral for the "isolated" resonance k is related to $J\left(\beta_k, \theta_k, a_k, 0\right)$ by

$$(RI)_k = \frac{\sigma_p}{E_{0k}} \Gamma_x \cdot c \cdot J\left(\beta_k, \theta_k, a_k, 0\right) , \tag{9}$$

where

$$c = 1 \quad \text{for resolved resonances}$$

$$= 1/\cos 2\delta_{\ell} \quad \text{for unresolved resonances}$$

In the multilevel formalism of the Adler-Adler form,[3,4] parameters are defined as follows:

$$\theta_k = \Gamma_k^{(s)}/\Delta \tag{10}$$

$$\nu_k = \Gamma_k^{(s)}/2 \tag{11}$$

$$a_k = (1/2)\left(H_{tk}/G_{tk}\right) \tag{12}$$

$$\beta_k = \sigma_p \cdot \Gamma_k^{(s)} \Big/ \left(4\pi\lambda^2 g_J G_{tk} \cdot \sqrt{E_{0k}}\right) \tag{13}$$

$$b_k = H_{xk}/G_{xk} \tag{14}$$

where the multilevel parameters are defined in Ref. 3 and obtained from ENDF/B by ETOE-2.

The corresponding resonance integral for an "isolated" resonance excluding the mutual self-shielding effect is therefore

$$(RI)_k = \frac{\sigma_p G_{xk}}{E_{0k}} \cdot \frac{\Gamma_k^{(s)}}{G_{tk}} \cdot J\left(\beta_k, \theta_k, a_k, b_k\right) . \tag{15}$$

With parameters for various cases defined, the numerical technique for evaluating $J\left(\beta_k, \theta_k, a_k, b_k\right)$ will be discussed. A direct numerical integration of Eq. (1) using any algorithm is highly undesirable due to the asymmetric behavior of the χ-function. The integration must be performed on the positive as well as the negative planes of x_k where the integrand

exhibits different behavior. However, this difficulty can be avoided and, in fact, one may take full advantage of the symmetric and the asymmetric properties of the ψ- and χ-functions by redefining $J\left(\beta_k,\theta_k,a_k,b_k\right)$ in the following way:

$$J\left(\beta_k,\theta_k,a_k,b_k\right) = J\left(\beta_k,\theta_k\right) + \int_0^\infty dx_k \sum_{n=1}^{\infty} \left(2a_k\right)^{2n} \frac{\psi\chi^{2n}}{\left(\beta_k+\psi\right)^{2n+1}}$$

$$- b_k \int_0^\infty dx_k \sum_{n=1}^{\infty} \left(2a_k\right)^{n} \frac{\chi^{2n}}{\left(\beta+\psi\right)^{2n}} . \qquad (16)$$

The two series in Eq. (16) must be uniformly convergent on physical grounds. Since $\left(\beta_k + 2a_k\chi + \psi\right)$ has the physical meaning of the total cross section which must be positive everywhere to be meaningful, it follows that $\beta_k + \psi \geq 2a_k\chi$ everywhere. It is interesting to note that the two geometric series can be written in closed form, and $J\left(\beta_k,\theta_k,a_k,b_k\right)$ becomes

$$J\left(\beta_k,\theta_k,a_k,b_k\right) = J\left(\beta_k,\theta_k\right) + I\left(\beta_k,\theta_k,a_k\right) - b_k \cdot M\left(\beta_k,\theta_k,a_k\right) , \qquad (17)$$

where the I- and M-integrals are defined as

$$I\left(\beta_k,\theta_k,a_k\right) = \left(2a_k\right)^2 \int_0^\infty \frac{\chi^2}{\left(\beta_k+\psi\right)^2 - \left(2a_k\chi\right)^2} \cdot \frac{\psi}{\beta_k+\psi}\, dx_k \qquad (18)$$

and

modulo different behavior. However, this difficulty can be avoided and, in fact, one may take full advantage of the symmetric and the asymmetric properties of the ψ- and χ-functions by redefining $\eta\left(\beta^X,\theta^X,\sigma^X,p^X\right)$ in the following way:

$$\eta\left(\beta^X,\theta^X,\sigma^X,p^X\right) = \eta\left(\beta^X,\theta^X\right) + \int_0^{\sigma^X} d\chi^X \sum_{n=1}^{\infty} \left(2\sigma^X\right)_{2n} \frac{\chi_{2n}}{\left(\beta^X+\theta\right)_{2n+1}}$$

$$- p^X \int_0^{\sigma^X} d\chi^X \sum_{n=1}^{\infty} \left(2\sigma^X\right)_p \frac{\chi_{2n}}{\left(\beta+\theta\right)_{2n}} \cdot \tag{18}$$

The two series in Eq. (18) must be uniformly convergent on physical grounds. Since $\left(\beta^X + 2\sigma^X\chi + \theta\right)$ has the physical meaning of the total cross section which must be positive everywhere to be meaningful; it follows that $\beta^X + \theta \geq 2\sigma^X\chi$ everywhere. It is interesting to note that the two geometric series can be written in closed form, and $\eta\left(\beta^X,\theta^X,\sigma^X,p^X\right)$ becomes

$$\eta\left(\beta^X,\theta^X,\sigma^X,p^X\right) = \eta\left(\beta^X,\theta^X\right) + I\left(\beta^X,\theta^X,\sigma^X\right) - p^X \cdot M\left(\beta^X,\theta^X,\sigma^X\right) \cdot \tag{17}$$

where the I- and M-integrals are defined as

$$I\left(\beta^X,\theta^X,\sigma^X\right) = \left(2\sigma^X\right)^2 \int_0^{\sigma^X} \frac{\chi^2}{\left(\beta^X+\theta\right)^2 - \left(2\sigma^X\chi\right)^2} \cdot \frac{\beta^X+\theta}{\pi}\, d\chi^X \tag{19}$$

and

$$M\left(\beta_k,\theta_k,a_k\right) = \left(2a_k\right)^2 \int_0^{\infty} \frac{\chi^2}{\left(\beta_k + \psi\right)^2 - \left(2a_k\chi\right)^2}\, dx_k \,. \qquad (19)$$

The advantage of Eq. (17) over Eq. (1) is quite obvious. Instead of integrating over both the positive and the negative planes of x_k, the integration now is over the positive x_k only. On the other hand, there are two extra integrals to be evaluated. It should be noted that the magnitudes of $I\left(\beta_k,\theta_k,a_k\right)$ and $M\left(\beta_k,\theta_k,a_k\right)$ are generally much smaller than that of the corresponding J-integral. For instance, in the case of the single-level formulation, a cursory check indicates that the magnitude of the I-integral is generally less than 15% of that of the corresponding J-integral for most cases of practical interest. A similar situation is also expected for the case of the multilevel formulation based on the limited data available on ^{235}U, ^{239}Pu, and ^{241}Pu. Hence, less strict error criteria are required for the I- and M-integrals.

An accurate and efficient algorithm using the Gauss-Jacobi quadrature[5] is proposed to evaluate these integrals simultaneously. In this algorithm, the J-integral is evaluated accurately to the relative error of less than 0.1% everywhere in the region of practical interest ($10^{-5} \leq \beta$; any θ. The same number of mesh-points are used for I- and M-integrals so that the total number of calculations for the ψ- and χ-integrals are minimized. The M- and I-integrals obtained this way are less accurate with the relative error of less than 1% which is believed to be sufficient for the problems of practical interest. The detailed description of this algorithm and its mathematical justification will be described in the following sections.

TECHNIQUE OF RATIONAL TRANSFORMATION

The proposed algorithm is directly based on the utilization of the general characteristics of the Gauss quadrature and the analytical behavior of the ψ- and χ-functions. In general, the efficiency of the Gauss quadrature depends strongly on how the integrand behaves. It is generally true that the integration is exact for a given number of mesh-points N if the integrand is of the form $\sum_k A_k x^k$ where $k \leq 2N - 1$. Clearly, the most favorable integrand for the Gauss-quadrature formulas[5] is the one which can be approximated by the polynomial $\sum_k A_k x^k$ with k as small as possible. As discussed previously,[1] the integrand of the form

$$\frac{\psi(x,\theta)}{\beta + \psi(x,\theta)}$$

does not meet this requirement since the ψ-function quickly approaches its asymptotic series when x becomes large. As one shall see later, the integrand of the form

$$\frac{\chi(\theta,x)}{\beta + \psi(\theta,x)}$$

is even worse since $\chi(\theta,x)$ approaches its asymptotic series faster than the corresponding $\psi(\theta,x)$. One way of resolving this problem is to divide the integrand into two parts whereby the integrand of the second integral in the asymptotic region also exhibits the form of $\sum_k A_k y^k$ with the variable of integration $y = 1/x$ as described by Ref. 6. In this report, a new method of treating integrands of the forms

$$\left(\frac{\psi}{\beta + \psi}\right)^n ,$$

$$\left(\frac{\chi}{\beta + \psi}\right)^{2n} ,$$

and

$$\left(\frac{\chi}{\beta + \chi}\right)^{2n}\left(\frac{\psi}{\beta + \psi}\right)$$

is proposed. For simplicity, let f(x) be the integrand under consideration. Instead of integration over x, a transformation is made so that

$$\int_0^\infty f(x)\,dx = \frac{1}{K}\int_0^1 \frac{du}{\sqrt{1 - u^2}}\,\frac{f(u)}{(1 - u^2)}$$

$$= \frac{\pi/N}{K}\left\{\frac{1}{2}\cdot f(0) + \sum_{i=2}^{(N-1)/2}\frac{f(u_i)}{1 - u_i^2}\right\} + R_N , \qquad (20)$$

where N, the total number of points over both the positive and the negative domains of u, is taken to be an odd integer and the new variable u is related to x by

$$u^2 = \frac{K^2x^2}{1 + K^2x^2} , \qquad (21)$$

and the choice of the parameter K will be discussed later.

Equation (2) represents the Gauss-Jacobi quadrature with odd number of mesh points where the related orthogonal polynomial is the Chebyshev polynomial of first kind and

$$u_i = \cos \frac{(2i - 1)\pi}{2N} \tag{22}$$

$$R_N = \frac{\pi}{(2N)!\ 2^{2N-1}} f^{(2N)}(\xi) \ ; \qquad 0 < \xi < 1 \ . \tag{23}$$

The inclusion of the $u_i = 0$ point is a significant saving in computing time since $\chi\left(0,\theta_k\right) = 0$ and $\psi\left(0,\theta_k\right)$ are related to the complementary error function which can be evaluated readily using the exceedingly efficient rational approximation suggested by Hastings.[7] Thus, the total number of entries to the ψ- and χ-functions is $(N - 1)/2$. The quantity $(N - 1)/2$ will be referred to as the total number of points required for the integration of all three integrals.

The purposes of making the rational transformation are many-fold. The most obvious purpose is to take advantage of the asymptotic properties of the ψ- and χ-functions whereby

$$\lim_{u \to 1} \left\{ \frac{1}{1 - u^2} \left(\frac{\psi}{\beta + \psi} \right) \right\} = \text{constant} \tag{24}$$

and

$$\lim_{u \to 1} \left\{ \frac{1}{1 - u^2} \left(\frac{\chi}{\beta + \psi} \right)^2 \right\} = \text{constant} \ . \tag{25}$$

Equation (2) represents the Gauss-Jacobi quadrature with odd number of mesh points where the related orthogonal polynomial is the Chebyshev polynomial of first kind and

$$\eta_i = \cos \frac{(2i - 1)\pi}{2N} \tag{22}$$

$$R_N = \frac{\pi}{(2N)!\, 2^{2N-1}} f^{(2N)}(\xi) \,, \quad 0 < \xi < 1 \,. \tag{23}$$

The inclusion of the $\eta_i = 0$ point is a significant saving in computing time since $\chi\left(0, s^N\right) = 0$ and $\epsilon\left(0, s^N\right)$ are related to the complementary error function which can be evaluated readily using the exceedingly efficient rational approximation suggested by Hastings.[7] Thus, the total number of entries to the ϕ- and χ-functions is $(N - 1)/2$. The quantity $(N - 1)/2$ will be referred to as the total number of points required for the integration of all three integrals.

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and

$$\lim_{u \to 1} \left\{ \frac{1}{1 - u_s^2} \left(\frac{\chi}{\beta + \theta} \right)^3 \right\} = \text{constant} \,. \tag{25}$$

Hence, the asymptotic behavior of $\sum_k a/x^k$ in the x domain can be eliminated. Of even greater importance from a mathematical point of view is that the transformation amounts to the analytic continuation of the series $\sum_{k=0}^{\infty} a_k x^k$ in the x domain which does not converge in the limit of large x. The corresponding series $\sum_k \gamma_k u^k$ is believed to converge much more rapidly in the u domain ($0 \leq u \leq 1$). By choosing the parameter K appropriately according to the analytical behavior of ψ- and χ-function, it was found that one may obtain an accuracy of 0.1% for the $J\left(\beta_k, \theta_k, 0, 0\right)$ integral and 1% or better for the I- and M-integrals using the same number of mesh points in the region of practical interest. The minimum number of mesh points required for the prescribed accuracy is obviously dependent on the magnitudes of β, θ, and a. For large θ, for instance, all integrals of the form defined in Eq. (17) are practically exact for a minimum of one point as ψ and χ become the natural line-shape functions. At the other extreme, a comparatively large number of mesh points is required when β and θ are both small. It was found that a total of six points is sufficient in all regions of practical interest.

The mathematical justification and the choice of the parameter will be given in the next section.

MATHEMATICAL JUSTIFICATION AND CHOICE OF K

In spite of the favorable numerical results in the preliminary investigations, mathematical justifications of the proposed method are needed. In order to illustrate the merits of the rational transformation, let

$$K = \sqrt{\frac{\beta}{\beta + A}}\, C \,, \tag{26}$$

where A and C are two arbitrary constants. If the ψ- and χ-functions assume the following forms

$$\psi \cong \frac{A}{1 + C^2x^2} \tag{27a}$$

and

$$\chi \cong \frac{AX}{1 + C^2x^2}, \tag{27b}$$

the integrands become

$$\frac{\psi/(\beta + \psi)}{1 - u^2} = 1 \tag{28}$$

and

$$\frac{\psi/(\beta + \psi)}{1 - u^2} \left[\frac{\chi}{(\beta + \psi)}\right]^{2N} = \text{constant} \cdot u^{2N} . \tag{29}$$

For the case of large θ, it is quite obvious that ψ- and χ-functions will approach the natural line shapes and the proposed method becomes the most efficient. For the case of small θ, the ψ- and χ-functions will approach the natural line-shape functions only if x is large. The rapidity with which the ψ- and χ- functions approach their asymptotic forms depends strongly on the magnitude of θ. Hence, the problem becomes the appropriate choice of K as a function of θ and β so that

$$f = \sum_{i=1}^{N} \alpha_i u_i^{2i} \tag{30}$$

converges rapidly in the non-asymptotic region where the ψ- and χ-functions are significantly different from their corresponding natural line shapes.

To further illustrate the problems involved, it is useful to examine some mathematical properties of ψ- and χ-integrals first.

A. Some Analytical Behavior of ψ- and χ-Functions

As mentioned previously, the merit of the proposed technique is rather obvious for the cases where θ is large. Hence, the cases with small θ will be emphasized. For small θ, it can be shown quite readily[4,8] that

$$\psi(0,x) = \int_0^\infty e^{-|\xi|-(\xi^2/\theta^2)} \cos x\xi \, d\xi$$

$$\simeq \frac{\sqrt{\pi}}{2} \theta \, e^{-y^2} - \frac{\theta^2}{2} \frac{dF(y)}{dy} + \cdots \tag{31}$$

$$\chi(\theta,x) = \int_0^\infty e^{-|\xi|-(\xi^2/\theta^2)} \sin x\xi \, d\xi$$

$$\simeq \theta F(y) - \frac{\sqrt{\pi}}{2} \theta^2 y \, e^{-y^2} + \cdots , \tag{32}$$

where

$$y = \frac{\theta}{2} x , \tag{33}$$

and F(y) is the Dawson integral defined as

$$F(y) = e^{-y^2} \int_0^y e^{t^2} \, dt . \tag{34}$$

The Dawson integral determines how rapidly ψ- and χ-integrals approach their asymptotic forms of $1/x^2$ and $1/x$ respectively. dF(y)/dy is related to F(y) in a simple way:

converges rapidly in the non-asymptotic region where the ψ- and χ-functions are significantly different from their corresponding natural line shapes.

To further illustrate the problems involved, it is useful to examine some mathematical properties of ψ- and χ-integrals first.

A. Some Analytical Behavior of ψ- and χ-Functions

As mentioned previously, the merit of the proposed technique is rather obvious for the cases where θ is large. Hence, the cases where θ/γ_D small ϵ will be emphasized. For small θ, it can be shown quite readily[29,30] that

$$\psi(\theta;x) = \int_0^\infty e^{-|\epsilon|-(\epsilon^2/\theta_2)} \cos x\epsilon \, d\epsilon$$

$$\simeq \frac{\sqrt{\pi}}{2} \theta \, e^{-\lambda_2} - \frac{\theta_2}{2} \frac{dF(\lambda)}{d\lambda} + \cdots \tag{31}$$

$$\chi(\theta;x) = \int_0^\infty e^{-|\epsilon|-(\epsilon^2/\theta_2)} \sin x\epsilon \, d\epsilon$$

$$\simeq \frac{\sqrt{\pi}}{2} \theta_2 \lambda \, e^{-\lambda_2} + \cdots , \tag{32}$$

where

$$\lambda = \frac{2}{\theta} x , \tag{33}$$

and $F(\lambda)$ is the Dawson integral defined as

$$F(\lambda) = e^{-\lambda_2} \int_0^\lambda e^{t_2} \, dt . \tag{34}$$

The Dawson integral determines how rapidly ψ- and χ-integrals approach their asymptotic forms of $1/x_2$ and $1/x$ respectively. $dF(\lambda)/d\lambda$ is related to $F(\lambda)$ in a simple way:

$$\frac{dF(y)}{dy} = 1 - 2yF(y) \ . \tag{35}$$

For small y, F(y) can be expressed as

$$F(y) = \sum_{k=0}^{\infty} \frac{(-1)^k 2^k y^{2k+1}}{1 \quad 3 \ . \ . \ . \ (2k+1)} \ , \tag{36}$$

and rapidly approaches its asymptotic series[9]

$$F(y) = \frac{1}{2y} + \sum_{k=1}^{\infty} \frac{1 \cdot 3 \ . \ . \ . \ (2k-1)}{2^{2k} y^{2k+1}} \ , \tag{37}$$

for $y > 1$. On the other hand, dF(y)/dy approaches its asymptotic series

$$\frac{dF(y)}{dy} = -\frac{1}{2y^2} - \sum_{k=1}^{\infty} \frac{1 \cdot 3 \ . \ . \ . \ (2k-1)}{2^{2k} y^{2k+2}} \cdot (2k+1) \ , \tag{38}$$

for $y \gg 1$. It is obvious that Eq. (37) converges much more rapidly than Eq. (38) for any given y.

For the ψ-integral, the Gaussian term is predominant when y is small, and the dF/dy term becomes more important when $y \geq \sim 3.5$ or larger depending on the magnitude of θ. For small y, the Gaussian term can be expressed as a power series

$$e^{-y^2} = \sum_{k=1}^{\infty} \frac{(-1)^k y^{2k}}{k!} \ . \tag{39}$$

For the χ-integral, the first term $\theta \cdot F(y)$ is always the predominant term as long as $\theta < 1$. By comparing the ratios of $(k+1)$-*th* and k-*th* terms in Eqs. (36), (37), (38), and (39), it is seen that the χ-function can be represented by a power series of y which converges approximately at the

same rate as the corresponding series of ψ-functions for small y and approaches the more rapidly converging asymptotic series when y becomes large. Hence, the region of convergence in the u-domain after the transformation is expected to be approximately the same for both ψ- and χ-functions. It is, therefore, reasonable to expect that

$$\frac{\chi^2}{(\beta + \psi)} = \sum_{i=0}^{\infty} \gamma_i u^{2i}$$

will converge reasonably rapidly as long as the corresponding

$$\frac{\psi}{\beta + \psi} = \sum_{i=0}^{\infty} \alpha_i u^{2i}$$

converges rapidly. This provides the basis for evaluating J-, M-, and I-integrals simultaneously using the same number of mesh points. One way of optimizing the quadrature formula defined in Eq. (20) is to choose an appropriate K so that the J-integral can be evaluated accurately; whereas the M- and I-integrals obtained using the identical mesh points will be less accurate depending on the magnitude of a_k as implied by Eq. (16).

There is yet another useful analytical behavior of ψ- and χ-functions. The optimization of Eq. (16) can also be pictured as a way to minimize the deviation of ψ- and χ-functions from the Lorentzian forms defined by Eqs. (27a) and (27b). In reality, with the exception of two extremes at small or large values of y, the deviation is generally large at intermediate values of y especially when θ becomes small. One way of minimizing the deviation of the ψ-function from Eq. 27a is to impose the condition

$$\int_0^\infty \left(\frac{A}{1 + c^2x^2} - \psi \right)^2 dx = 0 \tag{40}$$

or

$$\frac{A^2}{C} - \frac{2\sqrt{\pi}\,\theta}{C} e^{(\theta^2/4)(1+1/c)^2} \operatorname{Erfc}\left[\frac{\theta}{2} \left(1 + \frac{1}{c} \right) \right] A + \psi(0, \sqrt{2}\,\theta) = 0 \tag{41}$$

on the parameters A and C. Under this condition, Eq. (27a) is a good approximation in the least-square sense. It is interesting to note that the same relation is also true for the χ-function. It has been shown[8] that

$$\int_0^\infty \psi^2 \, dx = \int_0^\infty \chi^2 \, dx \, . \tag{42}$$

By using Parseval's theorem for the Fourier transforms,[10] it can be shown quite readily that

$$\int_0^\infty \frac{Ax}{1 + c^2x^2} \cdot \chi \, dx = \int_0^\infty \frac{A}{1 + c^2x^2} \psi \, dx \tag{43}$$

and

$$\int_0^\infty \left(\frac{Ax}{1 + c^2x^2} \right)^2 dx = \int_0^\infty \left(\frac{A}{1 + c^2x^2} \right)^2 dx \, . \tag{44}$$

Hence, the condition

$$\int_0^\infty \left(\frac{Ax}{1 + c^2x^2} - \chi \right)^2 dx = 0 \tag{45}$$

will also yield the same relation given by Eq. (41). Hence, the deviations of ψ- and χ-functions from the corresponding Lorentzian shapes are identical in the least-square sense.

B. Choice of Parameter K

The parameter K will be chosen to satisfy the error criteria of $|\varepsilon| \leq 0.1$ for J and $|\varepsilon| \leq 1\%$ for M- and I-integrals. Since the behavior of the integrand f and its derivatives $f^{(2n)}$ depend on the magnitudes of β and θ, it is, therefore, useful to divide the region of practical interest into three regions:

I. Fast Reactor Region $[\beta/\psi(0,\theta) \geq 0.2;\ \theta \leq 1]$

II. Lorentzian Region ($\theta > 0.5$ excluding Region I)

III. Intermediate Region (region excluding Regions I and II).

Figure 1 illustrates graphically the boundaries of these regions as a function of j and θ where $\beta = 2j \times 10^{-5}$. The choice of K in these three regions will be discussed as follows.

I. Fast Reactor Region $[\beta/\psi(0,\theta) \geq 0.2,\ \theta \leq 1]$

This region is extremely important for fast reactor calculations since approximately 80% or more of the resonances under consideration belong to this region. Two special characteristics of the integrands in this region are: (1) the shapes of the integrands are generally not too different from the corresponding ψ or χ^2 in the numerators; and (2) the integrands can always be expressed in terms of the rapidly convergent series in u. By utilizing these characteristics one may choose K using either one of the following arguments:

(1) On the Basis of Least-Squared Fitting - K can be chosen to satisfy Eq. (41). It is most convenient to set A = $\psi(0,\theta)$ and to solve for C from Eq. (41). By comparing the variations of the function of the Gauss form to that of the Lorentzian form, it is obvious that C must be less than $\theta/2$ in order to satisfy Eq. (41). For $C < \theta/2$, the second term in the transcendental equation becomes

$$\sqrt{\pi}\, e^{(\theta^2/4)(1+1/c)^2} \operatorname{Erfc}\left[\frac{\theta}{2}\left(1 + \frac{1}{c}\right)\right] \simeq \frac{1}{(\theta/2)(1 + 1/c)} . \qquad (46)$$

Hence, the solution is approximately

$$\frac{1}{c} = 2\left\{[1 - \psi(0,\theta)]\psi(0,\theta) - [\psi(0,\sqrt{2}\,\theta)/4] + \sqrt{\{[1 - \psi(0,\theta)]\psi(0,\theta) - [\psi(0,\sqrt{2}\,\theta)/4]\}^2 - [\psi^2(0,\theta)\psi(0,\sqrt{2}\,\theta)/4]}\right\} \Big/ \psi^2(0,\sqrt{2} \qquad (47)$$

where $\psi(0,\theta)$ and $\psi(0,\sqrt{2}\,\theta)$ can be evaluated most efficiently by using Hasting's rational approximation.[7]

(2) On the Basis of Analytic Continuation - The use of the analytic continuation argument yields a much simpler expression for K and is recommended over Eq. (47). Since the integrand of the form $\psi/(\beta + \psi)$ can always be expanded into a uniformly convergent series

$$\frac{\psi}{\beta + \psi} = \frac{\psi(x,\theta)}{\beta + \psi(0,\theta)} + \frac{\psi(x,\theta)[\psi(0,\theta) - \psi(x,\theta)]}{[\beta + \psi(0,\theta)]}$$

$$+ \frac{\psi(x,\theta)[\psi(0,\theta) - \psi(x,\theta)]^2}{[\beta + \psi(0,\theta)]^3} + \ldots . \qquad (48)$$

In the nonasymptotic region where $\psi(x,\theta)$ can be approximated by the Gauss-form, Eq. (48) becomes

$$\frac{\psi(x,\theta)}{\beta + \psi(x,\theta)} \simeq \frac{\psi(0,\theta)}{\beta + \psi(0,\theta)} \sum_{n=0}^{\infty} (-1)^n A_n y^{2n}$$

$$= \frac{\psi(0,\theta)}{\beta + \psi(0,\theta)} \left[1 + \sum_{n=1}^{\infty} B_n u^{2n}\right], \qquad (49)$$

where,

$$A_0 = 1 ;$$

$$A_1 = 1 - \frac{1}{\beta + \psi(0,\theta)} ;$$

$$A_2 = \frac{1}{2}\left[1 - \frac{3}{\beta + \psi(0,x)} - 2\psi(0,\theta) \cdot \left(\frac{1}{\beta + \psi(0,x)}\right)^2\right] ; \text{ etc.}$$

and

$$B_\nu = \left[\sum_{\lambda=1}^{\nu} (-1)^\lambda C_{\lambda-1}^{\nu-1} A_\lambda \cdot \frac{\theta^2}{4K^2}\right] \qquad (50)$$

$$C_{\lambda-1}^{\nu-1} = \frac{(\nu - 1)!}{(\nu - \lambda)!(\lambda - 1)!} \qquad \text{(the binomial coefficient).}$$

It was found that the convergence of Eq. (49) is relatively insensitive to the value of K as long as $\theta/6 \leq K \leq \theta/2$. From numerical experimentation, it was found that

$$K = \theta/5 \tag{51}$$

will yield the most accurate results in J-integral. A similar argument is also applicable to the M- and I-integrals. Equation (51) is much simpler than Eq. (47) and is therefore recommended.

It is interesting to note that K is independent of β in this region. It follows that the ψ- and χ-functions used in the integrals of a given β can be stored and used again for integrals with different β as long as θ is the same. This is particularly suitable for calculations of critical assemblies where the plates of the heavy isotopes may have different thickness and surroundings but the temperature stays the same.

It was found that five points or less are necessary to give the prescribed accuracy in this region.

II. Lorentzian Region ($\theta > 0.5$ Excluding Region I)

In this region, the ψ- and χ- function will approach their asymptotic form rapidly, and the quantity $\psi/(\beta + \psi)$ approaches $1/(\beta + 1 + \beta x^2)$ rapidly. Hence, K can be taken to be close to $\sqrt{\beta/(\beta + 1)}$. In this region, the accuracy of the integration is generally not sensitive to the values of K as long as $0.3\sqrt{\beta/(\beta + 1)} < K \leq \sqrt{\beta/(\beta + 1)}$. It was found

$$K \simeq \sqrt{2\beta/(\beta + 1)} \tag{52}$$

will generally give good results for J-, M-, and I-integrals.

As in the case of Region I, the proposed method is also exceedingly efficient in this region. Less than five points are required to give the prescribed accuracy.

III. Intermediate Region (Region Excluding Regions I and II)

Among the three regions, the proposed method is relatively least efficient in this one. It is the region where both β and θ are small. It is also the region of least importance in fast reactor applications.

For J-integral, the integrand $\psi/(\beta + \psi)$ exhibits a step function behavior with a sharp drop near

$$x = \frac{2}{\theta} \ln[2 + (\sqrt{\pi/2}\,\theta)/\beta] ,$$

where $\psi/(\beta + \psi)$ is approximately equal to half of the value at $x = 0$. This is quite obvious if ψ is replaced by the Gauss form. The point of inflection for $\psi/(\beta + \psi)$ is also close to this half-way point. Since the point of inflection is still small compared to $x = 7/\theta$ where $\psi(x,\theta)$ approaches $1/x^2$,[11] it is rather difficult to chose a K that will reproduce the same step function-like behavior for quantity $(1 - u^2)$.

One way of choosing K in this region is to use a reference point x_1, which represents the breaking point of the power series and the asymptotic series representations of $\psi/(\beta + \psi)$. The exact value of x_1 is extremely difficult to obtain. From Ref. 1 it is clear that x_1 must be approximately equal to the breaking point suggested by Nicholson and Grasseschi.[6] Hence, x_1 will be taken to be

$$x_1 = \frac{2}{\theta}\left[1.8971 + \ell n\left(1 + 0.85\,\frac{\sqrt{\pi}\,\theta}{2\beta}\right)\right]^{\frac{1}{2}} . \qquad (53)$$

for values of $x_1 \geq \sqrt{(\beta + 1)/\beta}$ and

$$x_1 = \left\{\frac{1}{2}\left\{\frac{4}{\theta^2}\left[1.8971 + \ell n\left(1 + 0.85 \cdot \frac{\sqrt{\pi}\,\theta}{2\beta}\right)\right] + \frac{1+\beta}{\beta}\right\}\right\}^{\frac{1}{2}} , \qquad (54)$$

for x_1 in Eq. (53) $< \sqrt{(\beta + 1)/\beta}$.

Define

$$u_1^2 = \frac{K^2 x_1^2}{1 + K^2 x_1^2} , \qquad (55)$$

so that

$$K^2 = \frac{u_1^2}{1 - u_1^2} \cdot \frac{1}{x_1^2} . \qquad (56)$$

By numerical experimentation, it was found that, by setting $u_1 \simeq 0.77$ or $1/K = 0.8292\, x_1$, good results in J-, M-, and I-integrals can be obtained for the case where Eq. (53) is valid. Better results can be obtained by letting

$$1/K = 0.8292\, x_1 \cdot \rho , \qquad (57)$$

where

$$\rho = 1 + \frac{0.018(\beta - 0.00128)}{\beta + 0.00128} + \frac{0.08\beta}{\psi(0,\theta)} . \qquad (58)$$

$$x_j = \frac{\theta}{2}\left[1.8921 + \ln\left(1 + 0.85\,\frac{\sqrt{\theta}}{2\theta}\right)\right]^2 . \tag{58}$$

for values of $x_j \geq \sqrt{(\theta + 1)/\theta}$ and

$$x_j = \left(\frac{2}{\pi}\left\{\frac{\theta_s}{4}\left[1.8921 + \ln\left(1 + 0.85\,\frac{\sqrt{\theta}}{2\theta}\right)\right] + \frac{1+\theta}{\theta}\right\}\right)^{\frac{1}{2}} . \tag{59}$$

for x_j in Eq. (53) $< \sqrt{(\theta + 1)/\theta}$.

Define

$$u_2^j = \frac{K_2 x_1^j}{1 + K_2 x_1^j} , \tag{60}$$

so that

$$K_2 = \frac{u_2^j}{1 - u_2^j} \cdot \frac{1}{x_1^j} . \tag{61}$$

By numerical experimentation, it was found that, by setting $u_1 \simeq 0.77$ or $1/K = 0.8292\ x_1$, good results in θ-, $1/K$-, and Γ-integrals can be obtained for the case where Eq. (53) is valid. Better results can be obtained by letting

$$1/K = 0.8292\ x_1 + \beta , \tag{57}$$

where

$$\beta = 1 + \frac{0.018(\theta - 0.00128)}{\theta + 0.00128} - \frac{0.08\theta}{\sqrt{(0.3)}} . \tag{58}$$

For the case where Eq. (54) is applicable, good results can be obtained by letting $u_1^2 = 0.5$ or

$$1/K = x_1 . \tag{59}$$

When β becomes extremely small, the integrands are not sensitive to the Gaussian-like behavior of ψ-function and Eq. (59) will approach the same limit defined previously for the Lorentzian region.

To give the prescribed accuracy of $|\varepsilon| \leq 0.1\%$ for the J-integral and $|\varepsilon| \leq 1\%$ for M- and I-integral, a total of six points is required in this region. It should be noted that Region III is generally very small for problems of practical interest. The cases with extremely small β are those for low-energy resonances with large neutron width. The combination of low resonance energy and large neutron width implies that θ must be reasonably large. It is extremely rare that a resonance will fall into the region $\beta \leq 10^{-3}$ and $\theta < 0.1$.

C. Further Economization

Under the condition that β_k is large compared to $\psi\left(0,\theta_k\right)$, $J\left(\beta_k,\theta_k,a_k,b_k\right)$ can be evaluated analytically without going through the integration routine. In fast reactor applications there are significantly large numbers of resonances that satisfy this condition. It is undoubtedly a significant saving on the computing time to include the analytical expressions in the proposed algorithm.

The integral $J\left(\beta_k,\theta_k,a_k,b_k\right)$ can be expressed in terms of a uniformly convergent series

$$J\left(\beta_k,\theta_k,a_k,b_k\right) = \frac{1}{2}\left\{\int_{-\infty}^{\infty} \frac{\psi\left(x_k,\theta_k\right) + b_k\chi\left(x_k,\theta_k\right)}{\beta_k + \psi\left(0,\theta_k\right)}\, dx_k \right.$$

$$+ \int_{-\infty}^{\infty} dx_k \frac{\left[\psi\left(x_k,\theta_k\right) + b_k\,\psi\left(x_k,\theta_k\right)\right]\left[\psi\left(0,\theta_k\right) - \psi\left(x_k,\theta_k\right) - 2a_k\chi\left(x_k,\theta_k\right)\right]}{\left[\beta_k + \psi\left(0,\theta_k\right)\right]^2}$$

$$\left. + \cdots \right\}$$

$$= \frac{\pi/2}{\left[\beta_k + \psi\left(0,\theta_k\right)\right]}\left\{1 + \frac{\left[\psi\left(0,\theta_k\right) - \frac{1}{2}\,\psi\left(0,\sqrt{2}\,\theta_k\right)\right] - a_k b_k \psi\left(0,\sqrt{2}\,\theta_k\right)}{\left[\beta_k + \psi\left(0,\theta_k\right)\right]}\right.$$

$$\left. + \cdots \right\}, \qquad (60)$$

where identities given by Eq. (43) were used. It was found that, for

$$\frac{\beta_k + \psi\left(0,\theta_k\right)}{\psi\left(0,\theta_k\right)} \geq 15 ,$$

an accuracy of $|\varepsilon| \leq 0.1\%$ can be obtained by keeping only the first two significant terms in Eq. (60). Thus,

$$J\left(\beta_k,\theta_k,0,0\right) \simeq \frac{\pi/2}{\left[\beta_k + \psi\left(0,\theta_k\right)\right]}\left[1 + \frac{\psi\left(0,\theta_k\right) - \frac{1}{2}\psi\left(0,\sqrt{2}\,\theta_k\right)}{\beta_k + \psi\left(0,\theta_k\right)}\right] \tag{61}$$

$$M\left(\beta_k,\theta_k,a_k\right) \simeq \frac{\frac{\pi}{2}a_k b_k \psi\left(0,\sqrt{2}\,\theta_k\right)}{\left[\beta_k + \psi\left(0,\theta_k\right)\right]^2} \tag{62}$$

$$I\left(\beta_k,\theta_k,a_k\right) \simeq 0 \,. \tag{63}$$

CONCLUSION

The new algorithm using the technique of the rational transformation and the Gauss-Jacobi quadrature is believed to provide an accurate, economical, and flexible tool for evaluting the $J\left(\beta_k,\theta_k,a_k,b_k\right)$ integral. This algorithm is particularly efficient in Region I where most of the practical problems in fast reactor applications belong and Region II where θ is relatively large. It was found that an accuracy of $|\varepsilon| \leq 0.1\%$ for the J-integral and $|\varepsilon| \leq 1.0\%$ for the M- and I-integrals can be obtained by using five mesh points or less (total entries of QUICKW routine).[12] For Region III, which is less important in fast reactor applications, six mesh points are required to give the prescribed accuracies. If one relaxes the accuracy of J-integral to $|\varepsilon| \leq 0.5\%$ for this region, five mesh points are sufficient. For MC^2-2, six points for all regions are recommended to avoid any inconvenience in the programming. FORTRAN listings are included in Appendix A.

$$\left[\frac{\pi\lambda^2}{\left[\beta^2 + \alpha\left(0,\theta^2\right)\right]^2}\right] \cdot \left[1 + \frac{\alpha\left(0,\theta^2\right) - \frac{1}{2}\,\alpha\left(0,\sqrt{2}\,\theta^2\right)}{\beta^2 + \alpha\left(0,\theta^2\right)}\right] \tag{B1}$$

$$\frac{\frac{\pi}{4}\,\alpha^2\beta^2\alpha\left(0,\sqrt{2}\,\theta^2\right)}{\left[\beta^2 + \alpha\left(0,\theta^2\right)\right]^2} \tag{B2}$$

$$\geq 0 \,. \tag{B3}$$

Since the integrand of the overlap integral in the resolved region exhibits a behavior similar to those for the J-, M-, and I-integrals, studies are under way to examine whether the same technique can be extended to the overlap integral.

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Since the integrand of the overlap integral in the resolved region exhibits a behavior similar to those for the δ-, N-, and I-integrals, studies are under way to examine whether the same technique can be extended to the overlap integral.

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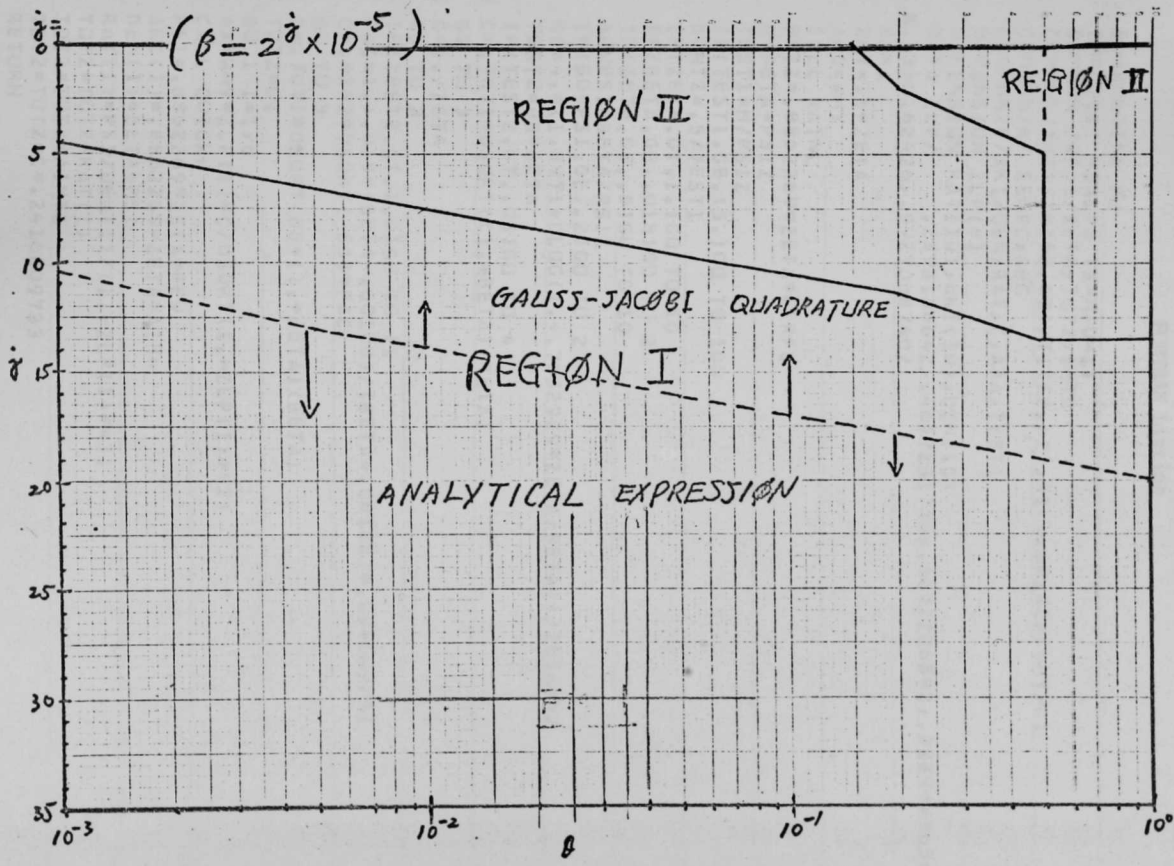
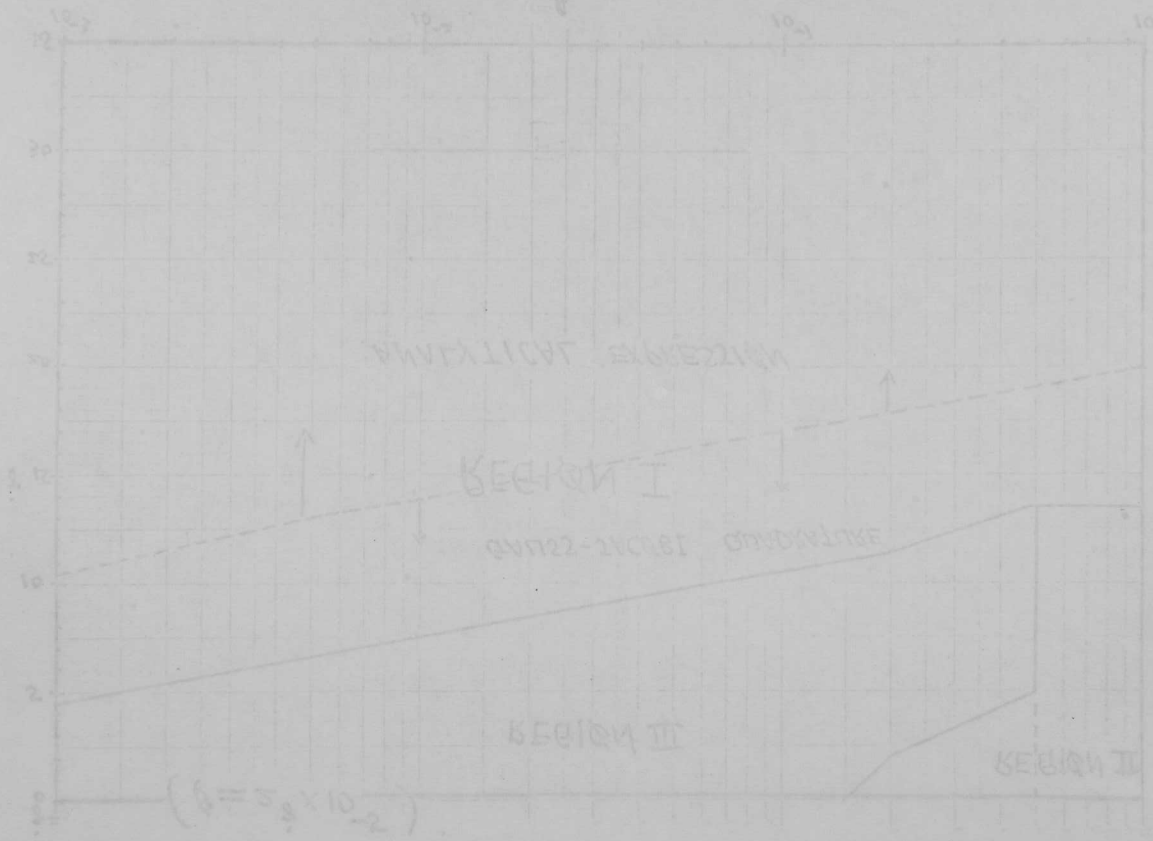


Fig. 1. Schematic illustration of various regions.



APPENDIX A

FORTRAN Listing

```
      SUBROUTINE FJ
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /QFJ1/ZETA,TOT2,BETA
      COMMON/TRTI/TR(62,62),TI(62,62),AIMW,AX,REW,WHY,KI
      COMMON/R/ EERFC,ARG
      COMMON/F/AKI,DEN,RAT,C,AAA,TEST1
      DIMENSION ZLP(8)
      DIMENSION RAT(10),AKI(10),DEN(10)
      DATA ZLP/     .2393156642,.4647231720,.6631226582,.8229838658,
     X.9350162426,.9927088740/
      KI=1
      WHY=.5*ZETA
      ARG=WHY
      CALL RATNL
      PSIZ=.8862269*ZETA*EERFC
      H=BETA+PSIZ
      TEST1=H/PSIZ
      IF(TEST1.GE.15.)GO TO 100
      AINTZ=.5/TEST1
      IF(ZETA.GT.1.)GO TO 10
      IF(BETA.GE..018)GO TO 2
      IF(ZETA.GE..5)GO TO 10
      BOVPSI=BETA/PSIZ
      IF(BOVPSI.GE..2)GO TO 2
      BB=4.*(1.8971+DLOG(1.+.7532929*ZETA/BETA))/ZETA**2
      TEST2=BB*BETA
      IF(TEST2.GT..03)GO TO 4
   10 C=.7071*DSQRT((1.+BETA)/BETA)
      GO TO 3
    2 C=5./ZETA
      GO TO 3
    4 IF(TEST2.LT.1.0)GO TO 11
      FAC=1.+.018*(BETA-.00128)/(BETA+.00128)+.08*BOVPSI
      C=.8292*DSQRT( BB)*FAC
      GO TO 3
   11 C=.7071*DSQRT(BB+(1.+BETA)/BETA)
    3 TOT2=0.
      DO 1 I=1,6
      AX=WHY*ZLP(I)*C/DSQRT(1.-ZLP(I)**2)
      CALL QUICKW
      PSI=.8862269*ZETA*REW
      AKI(I)=.8862269*ZETA*AIMW
      DEN(I)=BETA+PSI
      RAT(I)=PSI/DEN(I)/(1.-ZLP(I)**2)
    1 TOT2=TOT2+RAT(I)
      TOT2=TOT2+AINTZ
      TOT2=TOT2*C*.2416609733
      RETURN
  100 ARG=.707106781*ZETA
      CALL RATNL
      PSIZ2=.6266570686*ZETA*EERFC
      TOT2=1.57079632681*(1.+(PSIZ-PSIZ2)/H)/H
      RETURN
      END
```

```
      SUBROUTINE RATNL
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/R/ EERFC,ARG
      T=1./(1.+.47047*ARG)
      EERFC=.3480242*T-.0958798*T**2+.7478556*T**3
      RETURN
      END
```

```
      SUBROUTINE FI
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /QFJ1/ZETA,TOT2,BETA
      COMMON/TRTI/TR(62,62),TI(62,62),AIMW,AX,REW,WHY,KI
      COMMON/F/AKI,DEN,RAT,C,AAA,TEST1
      DIMENSION RAT(10),AKI(10),DEN(10)
      IF(TEST1.GE.15.)GO TO 100
      ASQ=AAA**2
      TOT2=0.0
      DO 1 I=1,6
      AKISQ=AKI(I)**2*ASQ
    1 TOT2=TOT2+(AKISQ/(DEN(I)**2-AKISQ))*RAT(I)
      TOT2=TOT2*C*.2416609733
      RETURN
  100 TOT2=0.
      RETURN
      END
```

B